

Abstract Submitted
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Calculated and Experimental Vibrational Properties of P700 and the Iron Sulfur Cluster in Photosystem I HARI LAMICHHANE, GARY HASTINGS, Georgia State University — Density functional theory (DFT) based vibrational frequency calculations of $\text{Fe}_4\text{S}_4(\text{SR})_4^{n-}$ clusters show that the intense iron-sulfur stretching modes lie in the frequency region between 300-400 cm^{-1} . Among them the iron-sulfur ligand (Fe-S^t) stretching modes are more intense and $\sim 30 \text{ cm}^{-1}$ lower in frequency than the iron-sulfur body (Fe-S^b) stretching modes. Calculations in tetrahydrofuran (THF) show that all these iron-sulfur stretching modes of vibration downshift by $\sim 20 \text{ cm}^{-1}$ upon reduction of the molecule. On the other hand, we have not observed any intense bands from chlorophyll a in the frequency region 400 to 320 cm^{-1} from the calculations. In an attempt to detect modes associated with iron sulfur clusters in PS I we have obtained light induced ($\text{P700}^+ - \text{P700}$) FTIR difference spectra for PSI particles from *S.6803* in the far infrared region. We observe difference bands at many frequencies in the 600-300 cm^{-1} region. Based on our calculations and literature values we claim that the negative bands at 388 cm^{-1} and 353 cm^{-1} in the ($\text{P700}^+ - \text{P700}$) FTIR difference spectra be assigned to Fe-S^b and Fe-S^t stretching modes of the ground state of the iron-sulfur cluster F_B .

Hari Lamichhane
Georgia State University

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